Phenol, 4-chloro-2-methoxy-16766-30-6 | DTXSID0074974

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 6.88

Global applicability domain: Inside

Local applicability domain index: 4.58e-01

Confidence level: 6.21e-01

Nearest Neighbors from the Training Set

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1,1,1-Trichloro-2-methyl-2-

propanol

Measured: 1.70 Predicted: 2.82

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Monolinuron

Measured: 14.1 Predicted: 9.06

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3-Chlorobenzyl alcohol

Measured: 19.5 Predicted: 7.92

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3-Chloroaniline Measured: 2.24 Predicted: 7.18

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2-Chloropyridine Measured: 19.1 Predicted: 6.11